1 Distribute fly ash phases

The user may create initial 3-D microstructures with a number of "generic" fly ash particles (see **Generate Initial Microstructure** submenu for details). The distribution of phases comprising fly ash particles may be accomplished within those generic fly ash particles, under one of two simplifying cases, by using this submenu. The form that appears is shown in Figure 1 (top of the form) and Figure 2 (bottom of the form).

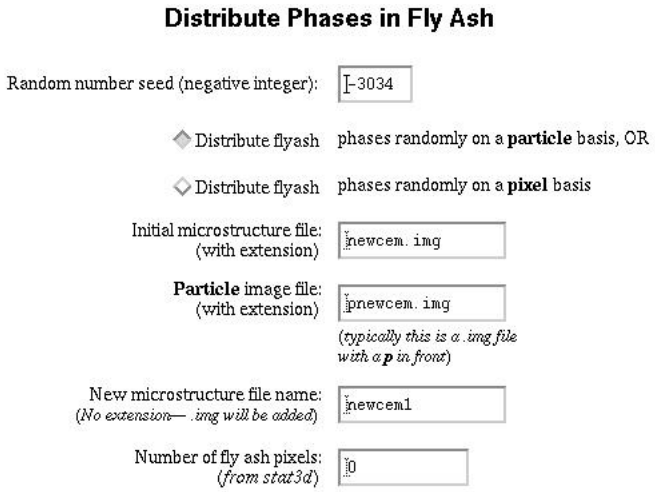

Figure 1: Top portion of the form for distributing fly ash phases within "generic" fly ash particles.

1.1 Random number seed

The user must enter a *negative integer* (in the range [-32767,-1]) in this field.

1.2 Method for distributing fly ash phases

The user has two choices:

1. **Particle basis**. Each particle is assumed to be comprised of a single phase, and the **particles** are randomly assigned phases to achieve a close approximation to the desired phase volume fractions specified in the table at the bottom of the form (see Figure 2). The program that executes this method is called `distfapart`.

2. **Pixel basis**. The phases are simply randomly distributed amongst all the generic fly ash *pixels* to achieve the volume fractions specified in the table at the bottom of the form (see Figure 2). This method produces a very fine and relatively uniform distribution of the fly ash phases within the individual particles. The program that executes this method is called `distfarand`.

1.3 Initial microstructure file

This must be the name of any 3-D microstructure image (extension `.img`) that contains generic fly ash particles.

1.4 Particle image file

This must be the name of the particle image file associated with the microstructure file already specified in the previous entry. For more information on the particle image file, see the **Generate 3D Microstructure** submenu. Because the same particle image file may be associated with any number of microstructure image files, this file name is requested separately instead of being automatically constructed from the name of the microstructure image file.

1.5 New microstructure file name

Enter the name that you wish the processed microstructure to have after this phase separation has been accomplished. As in previous forms already described, only the file root name should be supplied here; the extension `.img` will be added automatically.

1.6 Number of fly ash pixels

This number can be determined by computing the spatial statistics of the microstructure image, as described in the **Phase Statistics** submenu.

1.7 Phase fractions

Currently, the following phases are considered for distribution amongst the fly ash particles: aluminosilicate, calcium aluminodisilicate, silica, anhydrite, calcium chloride, tricalcium aluminate, and an inert phase. Reactions between these phases and the main components of cement have been incorporated into the current version of the cement hydration model [1, 2]. A warning message will appear if the user attempts to specify phase fractions the sum of which exceeds 1.0.

1.8 E-mail address

On most computers, either program `distfarand` or `distfapart` will execute within one minute. Nevertheless, the user has the option to specify an e-mail address to which an automatically-generated note will be sent upon completion of the calculation.

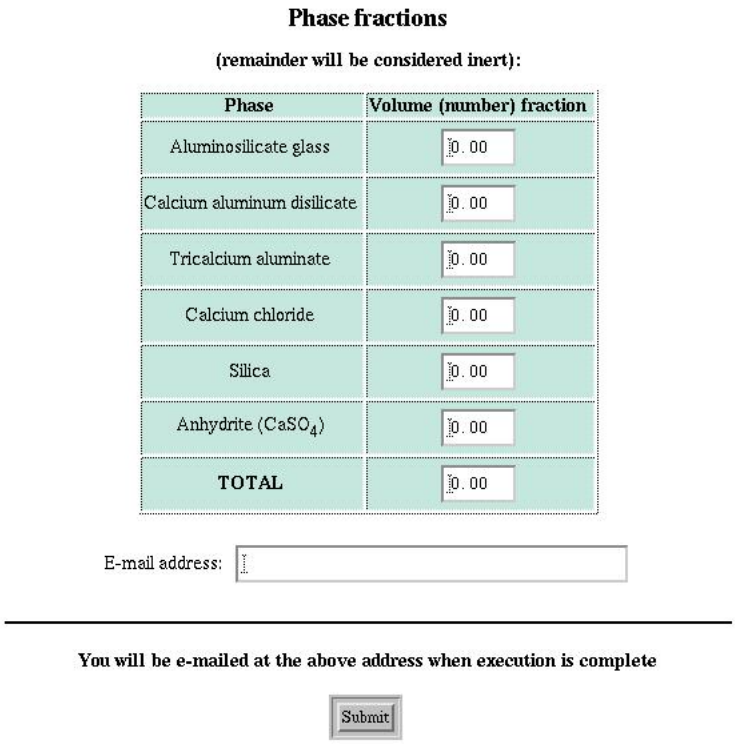

Figure 2: Bottom portion of the form for distributing fly ash phases within "generic" fly ash particles.

References

[1] D.P. Bentz. Cemhyd3d: A three-dimensional cement hydration and microstructural development modelling package. version 2.0. NISTIR 6485, U.S. Department of Commerce, April 2000.

[2] D.P. Bentz and S. Remond. Incorporation of fly ash into a 3-d cement hydration microstructure model. NISTIR 6050, U.S. Department of Commerce, August 1997. Available at http://ciks.cbt.nist.gov/∼bentz/flyash/flyash.html.